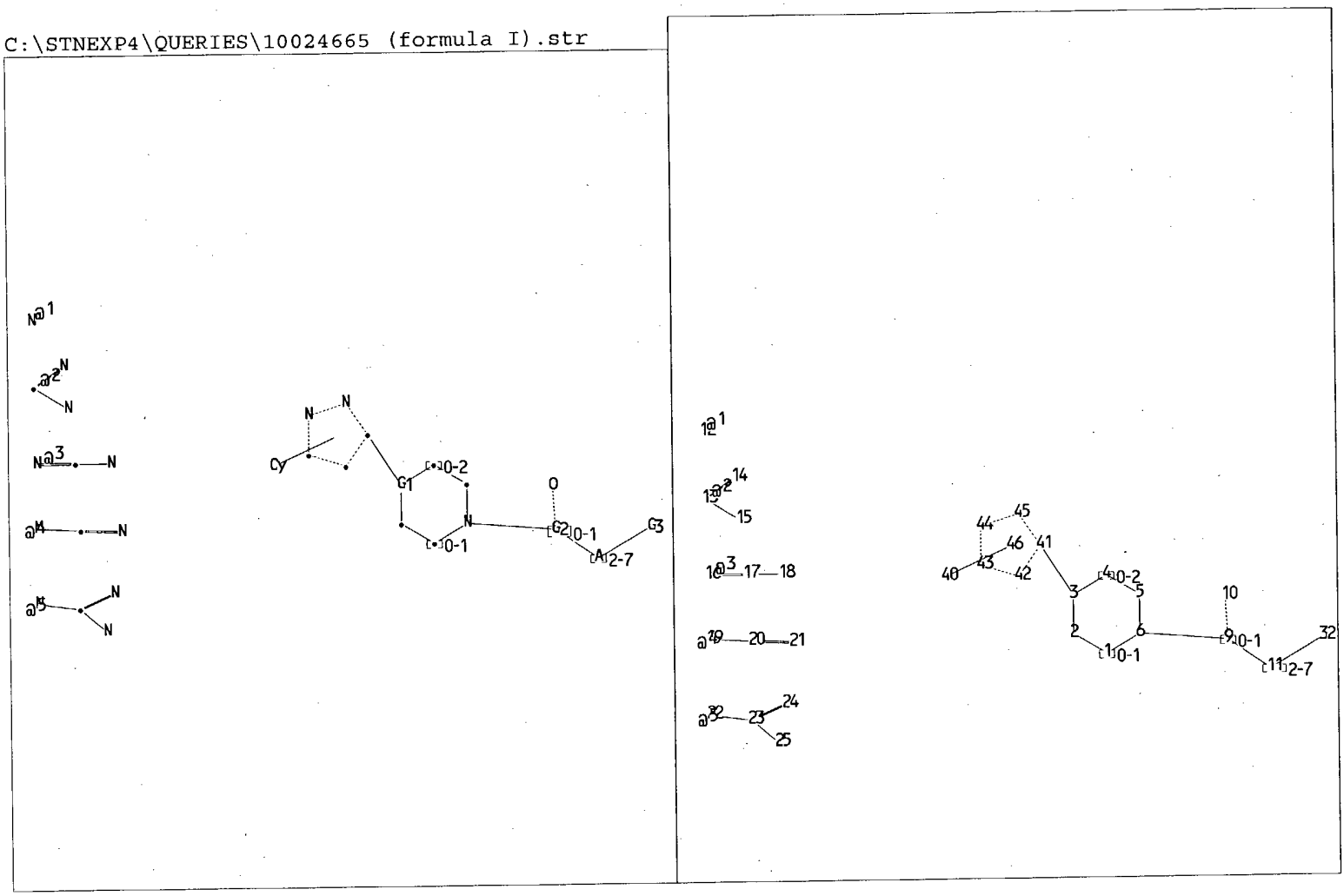
L Number	Hits	Search Text	DB	Time stamp
1	3591	((546/211) or (546/194) or (514/326) or (514/318)).CCLS.	USPAT; US-PGPUB; EPO; JPO; DERWENT	2004/02/03 18:20
2	2018146	2003.py. or 2004.py.	USPAT; US-PGPUB; EPO; JPO; DERWENT	2004/02/03 18:20
3	424	(((546/211) or (546/194) or (514/326) or (514/318)).CCLS.) and (2003.py. or 2004.py.)	USPAT; US-PGPUB; EPO; JPO; DERWENT	2004/02/03 18:20

C:\STNEXP4\QUERIES\10024665 (formula I).str



chain nodes :
9 10 11 16 32 40
ring nodes :
1 2 3 4 5 6 41 42 43 44 45
ring/chain nodes :
12 13 14 15 17 18 19 20 21 22 23 24 25
chain bonds :
3-41 6-9 9-11 9-10 11-32 13-14 13-15 16-17 17-18 19-20 20-21 22-23 23-24 23-25
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 41-42 41-45 42-43 43-44 44-45
exact/norm bonds :
1-2 1-6 2-3 3-4 3-41 4-5 5-6 6-9 9-11 9-10 11-32 13-14 13-15 16-17 17-18
19-20 20-21 22-23 23-24 23-25 41-42 41-45 42-43 43-44 44-45
isolated ring systems :
containing 1 : 41 :

G1:C,N

G2:C,S

G3:Cy,[*1],[*2],[*3],[*4],[*5]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 9:CLASS 10:CLASS 11:CLASS 12:CLASS
13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS
22:CLASS 23:CLASS 24:CLASS 25:CLASS 32:CLASS 40:Atom 41:CLASS 42:CLASS 43:CLASS
44:Atom 45:CLASS 46:CLASS
Generic attributes :
40:
Saturation : Unsaturated
Number of Carbon Atoms : less than 7

Number of Hetero Atoms : less than 2
Type of Ring System : Monocyclic

Element Count :
Node 40: Limited
C,C4-6
O,O0
S,S0
N,N0-1

```
=>
Uploading
THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE
Do you want to switch to the Registry File?
Choice (Y/n):
Switching to the Registry File...
Some commands only work in certain files.  For example, the EXPAND
command can only be used to look at the index in a file which has an
index.  Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of
commands which can be used in this file.

=> FILE REGISTRY

COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.42       0.42

FILE 'REGISTRY' ENTERED AT 18:00:25 ON 03 FEB 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:    2 FEB 2004  HIGHEST RN 645336-91-0
DICTIONARY FILE UPDATES:   2 FEB 2004  HIGHEST RN 645336-91-0

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading 10024665 (formula i).str

L1      STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.


=> s l1 sss sam
SAMPLE SEARCH INITIATED 18:00:51 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -  18055 TO ITERATE
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  5.5% PROCESSED    1000 ITERATIONS                                0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       353062 TO   369138
PROJECTED ANSWERS:               0 TO        0

L2            0 SEA SSS SAM L1

=> s l1 sss ful
FULL SEARCH INITIATED 18:01:01 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 359439 TO ITERATE

100.0% PROCESSED  359439 ITERATIONS                             31 ANSWERS
SEARCH TIME: 00.00.05

L3           31 SEA SSS FUL L1

=> s l3
L4           10 L3

=> d l4 1-10 bib,ab,hitstr
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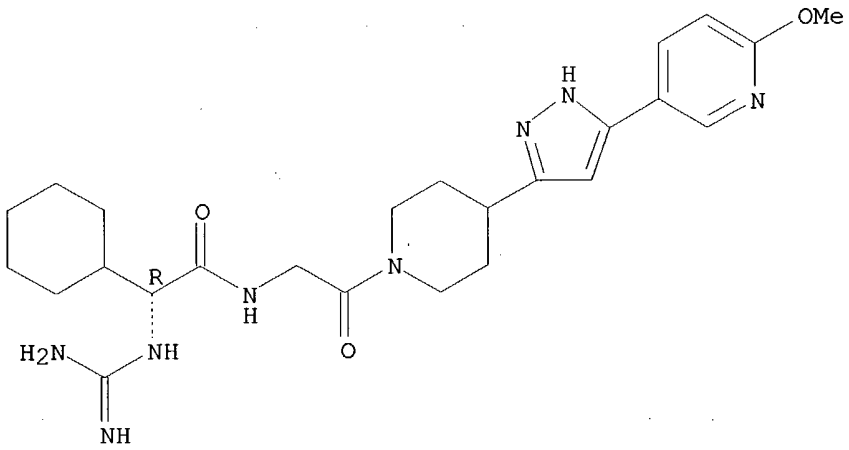
L4 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2003:491149 CAPLUS
DN 139:69524
TI Preparation of small-molecule inhibitors of interleukin-2
IN Arkin, Michelle R.; McDowell, Robert S.; Oslob, Johan D.; Raimundo, Brian C.; Waal, Nathan D.; Yu, Chul Hyun
PA Sunesis Pharmaceuticals, Inc., USA
SO PCT Int. Appl., 98 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

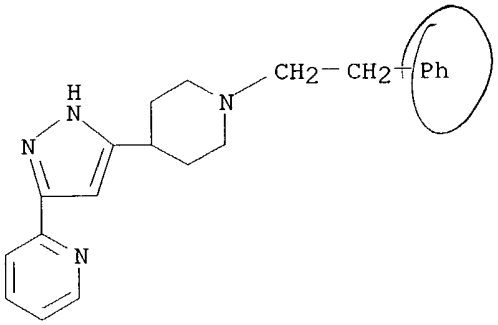
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2003051797	A2	20030626	WO 2002-US40430	20021217
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2003149049	A1	20030807	US 2001-24665	20011217
PRAI US 2001-24665	A	20011217		

OS MARPAT 139:69524
AB The invention describes compds. I [B = CH2CH2, CH2CH2NH, CH2OCH2, CONH, CO, SO, SO2NH, etc.; J = absent, S, CH2O, NH, CO, etc.; B = amino, amidino, (un)substituted Ph, naphthyl, cycloalkyl, heterocyclyl, etc.; A = N or CH; X = null, CH2 or CH2CH2, which may be substituted; Y = null or CH2; R = (un)substituted Ph, pyridyl, cyclopentadienyl, pyrrolyl, furyl, or thienyl; R1 = H, alkyl, haloalkyl, cycloalkyl; R2 = H and R3 = H, (cyclo)alkyl, halo, alkoxy, etc. or CR2R3 = CO; R4 = H, OH, alkoxy, (cyclo)alkyl, halo, haloalkyl] and amino acid derivs. II [same B, J, and M; R5 = (un)substituted phenyl; R6, R7 = H, CN, NO2, Ph, PhO, PhCH2, (cyclo)alkyl, etc.; R8 = H, (cyclo)alkyl, aryl, acetylaminoalkyl, etc.] which IL-2/IL-2R binding and are useful for the treatment of interleukin-2 mediated diseases, such as autoimmune diseases (such as rheumatoid arthritis, multiple sclerosis, uveitis, and psoriasis), allograft rejection, and graft-vs.-host disease. Thus, H2NC(:NH)-D-Ala-Gly-(4-PhC.tplbond.C-L-Phe)-OMe was prepd. coupling/deprotection reactions of 4-phenylethynyl-substituted phenylalanine Me ester hydrochloride with Boc-glycine (Boc = tert-butoxycarbonyl), Boc-D-alanine, and 1-pyrazolyl-C(:NBoc)NHBoc.
IT **550377-14-5P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of small-mol. inhibitors of interleukin-2)
RN 550377-14-5 CAPLUS
CN Cyclohexaneacetamide, .alpha.-[(aminoiminomethyl)amino]-N-[2-[4-[5-(6-methoxy-3-pyridinyl)-1H-pyrazol-3-yl]-1-piperidinyl]-2-oxoethyl]-, (.alpha.R)- (9CI) (CA INDEX NAME)

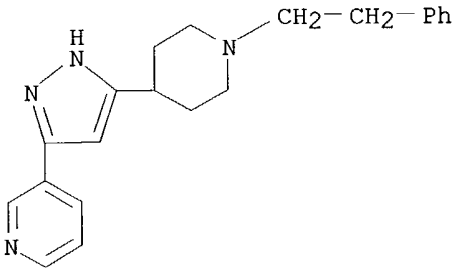
Absolute stereochemistry.


OMe
H
N
N
N
R
O
N
H
N
O
H_2N
NH
NH

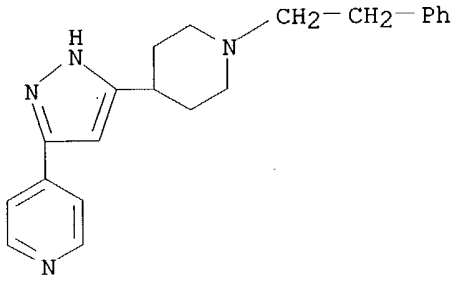
L4 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2003:333277 CAPLUS
DN 139:62616
TI A 3D QSAR Study on a Set of Dopamine D4 Receptor Antagonists
AU Bostroem, Jonas; Boehm, Markus; Gundertofte, Klaus; Klebe, Gerhard
CS H. Lundbeck A/S, Copenhagen-Valby, DK-2500, Den.
SO Journal of Chemical Information and Computer Sciences (2003), 43(3), 1020-1027
CODEN: JCISD8; ISSN: 0095-2338
PB American Chemical Society
DT Journal
LA English
AB The mol. alignments obtained from a previously reported pharmacophore model have been employed in a three-dimensional quant. structure-activity relationship (3D QSAR) study, to obtain a more detailed insight into the structure-activity relationships for D2 and D4 receptor antagonists. The frequently applied CoMFA method and the related CoMSIA method were used. Statistically significant models have been derived with these two methods, based on a set of 32 structurally diverse D2 and D4 receptor antagonists. The CoMSIA and the CoMFA methods produced equally good models expressed in terms of q2 values. The predictive power of the derived models were demonstrated to be high. Graphical interpretation of the results, provided by the CoMSIA method, brings to light important structural features of the compds. related to either low- or high-affinity D2 or D4 antagonism. The results of the 3D QSAR studies indicate that bulky N-substituents decrease D2 binding, whereas D4 binding is enhanced. Electrostatically favorable and unfavorable regions exclusive to D2 receptor binding were identified. Likewise, certain hydrogen-bond acceptors can be used to lower D2 affinity. These observations may be exploited for the design of novel dopamine D4 selective antagonists.
IT **156337-22-3 184374-56-9 184374-60-5**
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(3D QSAR study on set of dopamine D4 receptor antagonists)
RN 156337-22-3 CAPLUS
CN Pyridine, 2-[5-[1-(2-phenylethyl)-4-piperidinyl]-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



RN 184374-56-9 CAPLUS
CN Pyridine, 3-[5-[1-(2-phenylethyl)-4-piperidinyl]-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



RN 184374-60-5 CAPLUS
CN Pyridine, 4-[5-[1-(2-phenylethyl)-4-piperidinyl]-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



RE.CNT 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2003:150531 CAPLUS
DN 138:187765
TI Preparation of heteroarylpyrazoles as p38 kinase inhibitors
IN Anantanarayan, Ashok; Clare, Michael; Collins, Paul W.; Crich, Joyce Zuowu; Devraj, Rajesh; Flynn, Daniel L.; Geng, Lifeng; Graneto, Matthew J.; Hanau, Cathleen E.; Hanson, Gunnar J.; Hartmann, Susan J.; Hepperle, Michael; Huang, He; Koszyk, Francis J.; Liao, Shuyuan; Metz, Suzanne; Partis, Richard A.; Perry, Thao D.; Rao, Shashidhar N.; Selness, Shaun Raj; South, Michael S.; Stealey, Michael A.; Talley, John Jeffrey; Vazquez, Michael L.; Weier, Richard M.; Xu, Xiangdong; Khanna, Ish K.; Yu, Yi
PA G.D. Searle and Co., USA
SO U.S., 415 pp., Cont.-in-part of U.S. Ser. No. 196,623.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 4

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 6525059	B1	20030225	US 2000-513351	20000224
US 6514977	B1	20030204	US 1998-196623	19981120
WO 2000031063	A1	20000602	WO 1999-US26007	19991117

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RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRAI	US 1998-196623	A2	19981120
	WO 1999-US26007	A1	19991117
	US 1997-47570P	P	19970522
	US 1998-83670	A2	19980522

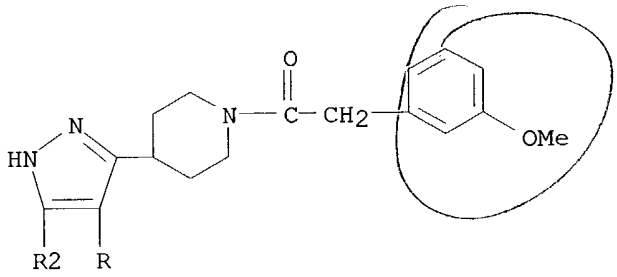
OS MARPAT 138:187765
AB Title compds. [I; R1 = H, OH, NH2, (cyclo)alk(en)yl, acyl, aryl, etc.; R2 = (un)substituted piperidinyl; R3 = (un)substituted pyrimidinyl; R4 = (un)substituted Ph; and pharmaceutically acceptable salts or tautomers thereof] were prepd. by soln. phase and solid phase parallel array reactions of ketones with hydrazines. Thus, R3CH2COMe (R3 = 4-pyridinyl) was condensed with 3,4-F(MeO)C6H3CHO to give the butenone (80%), which was cyclocondensed with TsNHNH2 to afford the title compd. II (20.7%). The latter inhibited human p38 kinase activity in vitro with IC50 of 4.6 .mu.M and inhibited tumor necrosis factor .alpha. (TNF.alpha.) and interleukin 1.beta. (IL-1.beta.) release from human peripheral blood mononuclear cells following stimulation with lipopolysaccharide with IC50 of 0.5 .mu.M. Thus, I are useful for the treatment of inflammation, arthritis, asthma, and other disorders mediated by p38 kinase and TNF.alpha..
IT **216523-75-0P 216523-79-4P 216523-84-1P**
216523-85-2P 216523-87-4P 216524-32-2P
216524-96-8P 216525-00-7P 216525-02-9P
216525-57-4P 216525-69-8P 216525-71-2P
216525-72-3P 271576-62-6P
RL: CPN (Combinatorial preparation); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); CMBI (Combinatorial study); PREP (Preparation); USES (Uses)

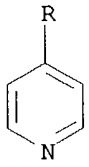
(p38 kinase inhibitor; prepn. of heteroarylpyrazole p38 kinase inhibitors by cyclocondensation of hydrazines with ketones)

RN 216523-75-0 CAPLUS

CN Piperidine, 4-[5-(4-fluorophenyl)-4-(4-pyridinyl)-1H-pyrazol-3-yl]-1-[(3-methoxyphenyl)acetyl]- (9CI) (CA INDEX NAME)

PAGE 1-A





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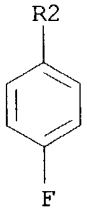
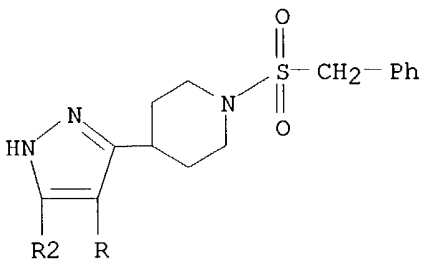
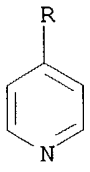


RN 216523-79-4 CAPLUS

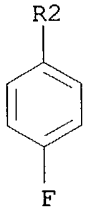
CN Piperidine, 4-[5-(4-fluorophenyl)-4-(4-pyridinyl)-1H-pyrazol-3-yl]-1-[(phenylmethyl)sulfonyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



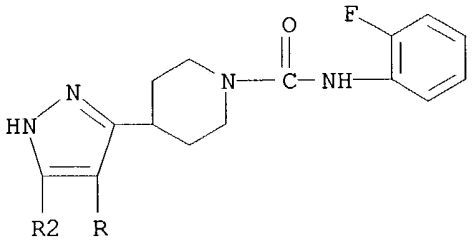


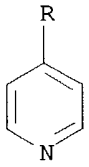
PAGE 2-A



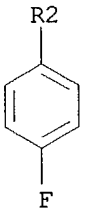
RN 216523-84-1 CAPLUS
CN 1-Piperidinecarboxamide, N-(2-fluorophenyl)-4-[5-(4-fluorophenyl)-4-(4-pyridinyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

PAGE 1-A



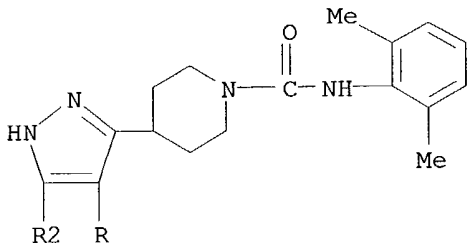


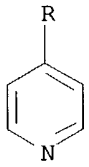
PAGE 2-A



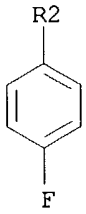
RN 216523-85-2 CAPLUS
CN 1-Piperidinecarboxamide, N-(2,6-dimethylphenyl)-4-[5-(4-fluorophenyl)-4-(4-pyridinyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

PAGE 1-A



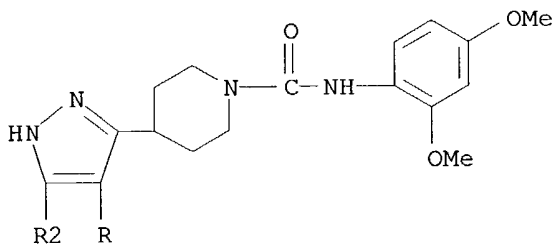


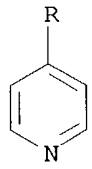
PAGE 2-A



RN 216523-87-4 CAPLUS
CN 1-Piperidinecarboxamide, N-(2,4-dimethoxyphenyl)-4-[5-(4-fluorophenyl)-4-(4-pyridinyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

PAGE 1-A





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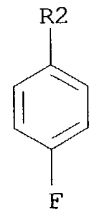
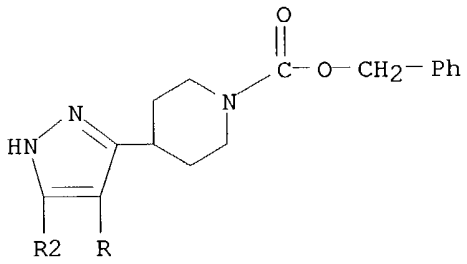
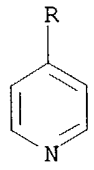


RN 216524-32-2 CAPLUS
CN 1-Piperidinecarboxylic acid, 4-[5-(4-fluorophenyl)-4-(4-pyridinyl)-1H-pyrazol-3-yl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A





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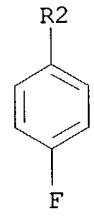
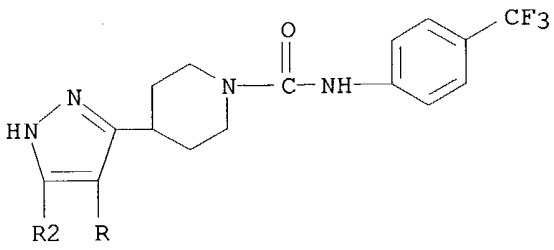
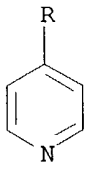


RN 216524-96-8 CAPLUS
CN 1-Piperidinecarboxamide, 4-[5-(4-fluorophenyl)-4-(4-pyridinyl)-1H-pyrazol-3-yl]-N-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

PAGE 1-A





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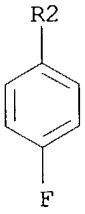

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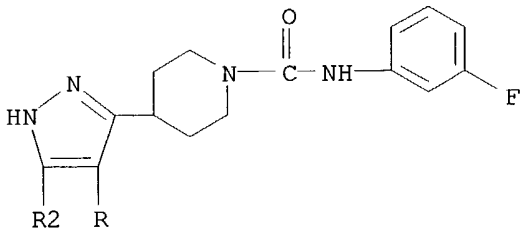
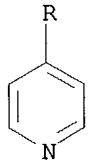
CN 1-Piperidinecarboxamide, N-(3-fluorophenyl)-4-[5-(4-fluorophenyl)-4-(4-pyridinyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

PAGE 1-A





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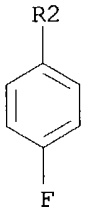
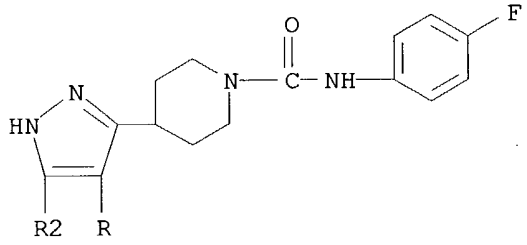
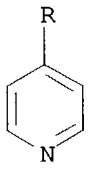


RN 216525-02-9 CAPLUS
CN 1-Piperidinecarboxamide, N-(4-fluorophenyl)-4-[5-(4-fluorophenyl)-4-(4-pyridinyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

PAGE 1-A





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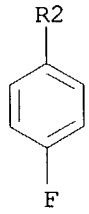

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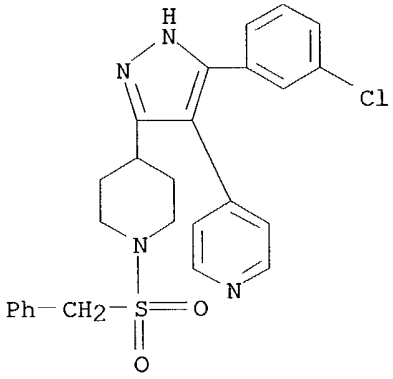

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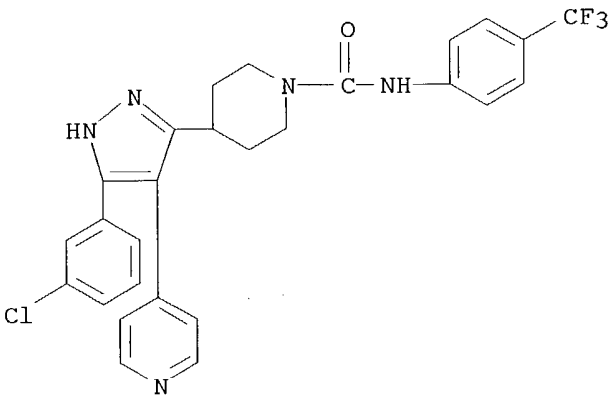

RN 216525-71-2 CAPLUS
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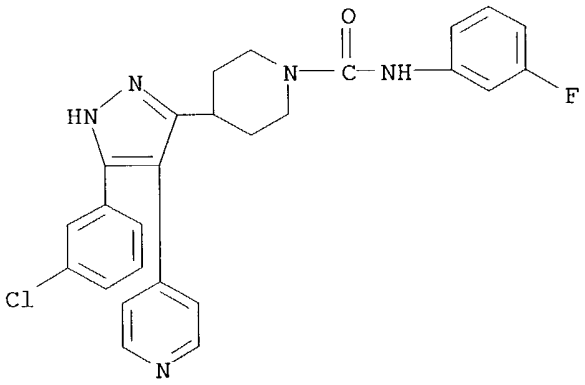

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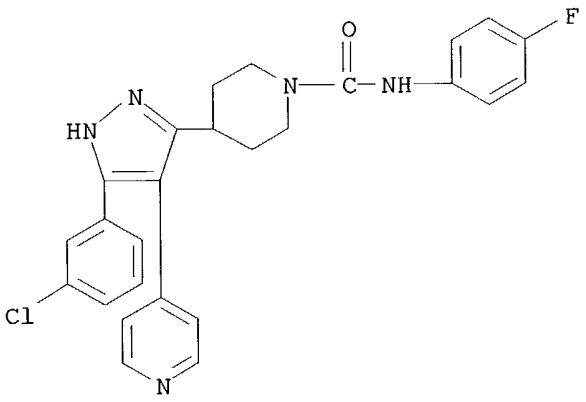

RN 271576-62-6 CAPLUS
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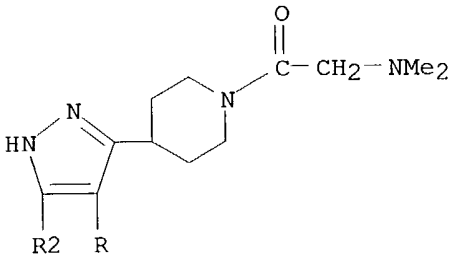
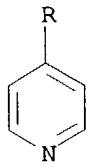
PAGE 1-A





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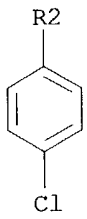

RE.CNT 75 THERE ARE 75 CITED REFERENCES AVAILABLE FOR THIS RECORD

L4 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2003:92403 CAPLUS
DN 138:137307
TI Preparation of heteroarylpyrazoles as p38 kinase inhibitors
IN Anantanarayan, Ashok; Clare, Michael; Collins, Paul W.; Crich, Joyce Zuowu; Devraj, Rajesh; Flynn, Daniel L.; Geng, Lifeng; Graneto, Matthew J.; Hanau, Cathleen E.; Hanson, Gunnar J.; Hartmann, Susan J.; Hepperle, Michael; Huang, He; Koszyk, Francis J.; Liao, Shuyuan; Metz, Suzanne; Partis, Richard A.; Perry, Thao D.; Rao, Shashidhar N.; Selness, Shaun Raj; South, Michael S.; Stealey, Michael A.; Talley, John Jeffrey; Vazquez, Michael L.; Weier, Richard M.; Xu, Xiangdong; Khanna, Ish K.; Yu, Yi
PA G.D. Searle and Co., USA
SO U.S., 541 pp., Cont.-in-part of U.S. Ser. No. 83,670.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 4

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OS MARPAT 138:137307
AB Title compds. [I; R1 = H, OH, NH2, (cyclo)alk(en)yl, acyl, aryl, etc.; R2 = (un)substituted piperidinyl or piperazinyl; R3 = (un)substituted pyrimidinyl; R4 = (un)substituted Ph; and pharmaceutically acceptable salts or tautomers thereof] were prepd. by soln. phase and solid phase parallel array reactions of ketones with hydrazines. Thus, R3CH2COMe (R3 = 4-pyridinyl) was condensed with 3,4-F(MeO)C6H3CHO to give the butenone (80%), which was cyclocondensed with TsNHNH2 to afford the title compd. II (20.7%). The latter inhibited human p38 kinase activity in vitro with IC50 of 4.6 .mu.M and inhibited tumor necrosis factor .alpha. (TNF.alpha.)

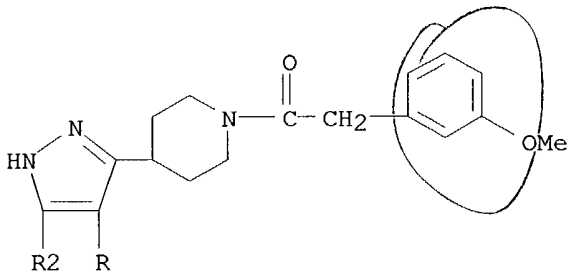
and interleukin 1.beta. (IL-1.beta.) release from human peripheral blood mononuclear cells following stimulation with lipopolysaccharide with IC50 of 0.5 .mu.M. Thus, I are useful for the treatment of inflammation, arthritis, asthma, and other disorders mediated by p38 kinase and TNF.alpha..

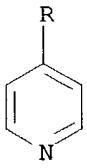
IT **216523-75-0P 216523-79-4P 216523-84-1P**
216523-85-2P 216523-87-4P 216524-32-2P
216524-96-8P 216525-00-7P 216525-02-9P
216525-57-4P 216525-69-8P 216525-71-2P
216525-72-3P 271576-62-6P
RL: CPN (Combinatorial preparation); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); CMBI (Combinatorial study); PREP (Preparation); USES (Uses)
(p38 kinase inhibitor; prepn. of heteroarylpyrazole p38 kinase inhibitors by cyclocondensation of hydrazines with ketones)

RN 216523-75-0 CAPLUS

CN Piperidine, 4-[5-(4-fluorophenyl)-4-(4-pyridinyl)-1H-pyrazol-3-yl]-1-[(3-methoxyphenyl)acetyl]- (9CI) (CA INDEX NAME)

PAGE 1-A





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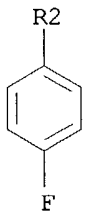

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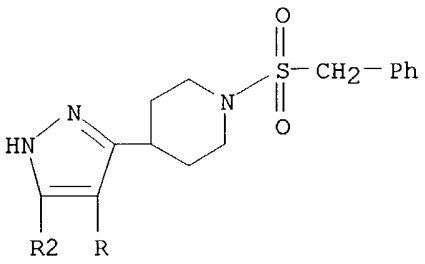
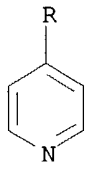
CN Piperidine, 4-[5-(4-fluorophenyl)-4-(4-pyridinyl)-1H-pyrazol-3-yl]-1-[(phenylmethyl)sulfonyl]- (9CI) (CA INDEX NAME)

PAGE 1-A





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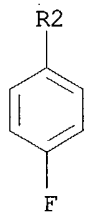
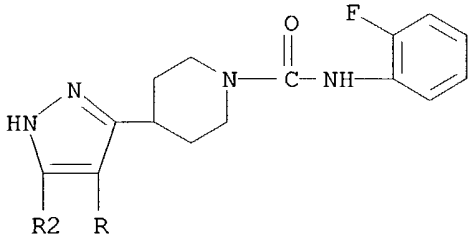
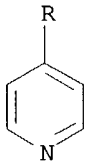


RN 216523-84-1 CAPLUS
CN 1-Piperidinecarboxamide, N-(2-fluorophenyl)-4-[5-(4-fluorophenyl)-4-(4-pyridinyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

PAGE 1-A





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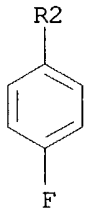

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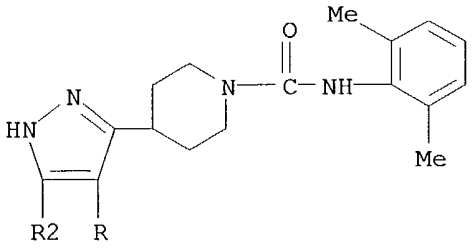
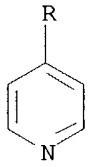
CN 1-Piperidinecarboxamide, N-(2,6-dimethylphenyl)-4-[5-(4-fluorophenyl)-4-(4-pyridinyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

PAGE 1-A





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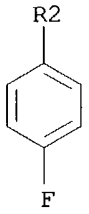

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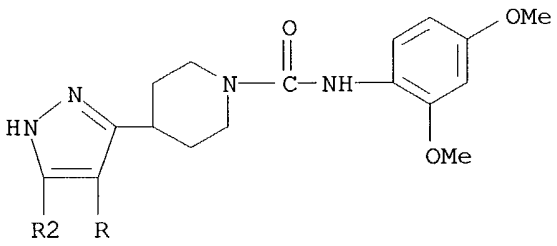
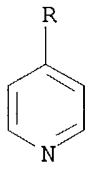
CN 1-Piperidinecarboxamide, N-(2,4-dimethoxyphenyl)-4-[5-(4-fluorophenyl)-4-(4-pyridinyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

PAGE 1-A





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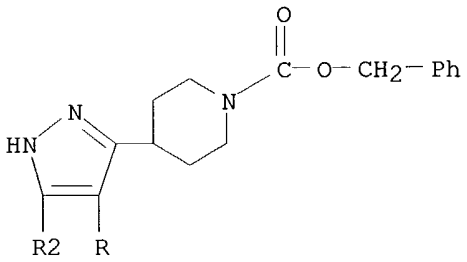
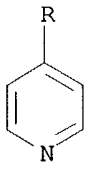
RN 216524-32-2 CAPLUS
CN 1-Piperidinecarboxylic acid, 4-[5-(4-fluorophenyl)-4-(4-pyridinyl)-1H-pyrazol-3-yl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A





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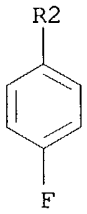

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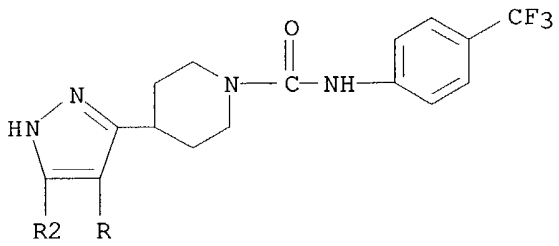
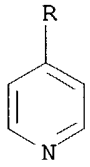
CN 1-Piperidinecarboxamide, 4-[5-(4-fluorophenyl)-4-(4-pyridinyl)-1H-pyrazol-3-yl]-N-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

PAGE 1-A





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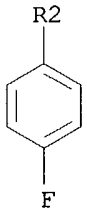
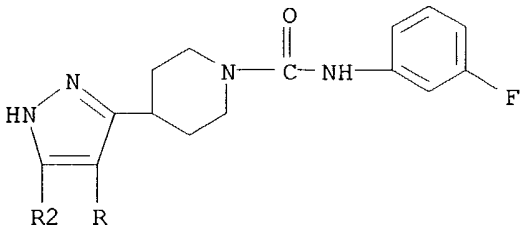
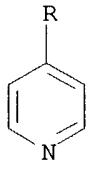


RN 216525-00-7 CAPLUS
CN 1-Piperidinecarboxamide, N-(3-fluorophenyl)-4-[5-(4-fluorophenyl)-4-(4-pyridinyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

PAGE 1-A





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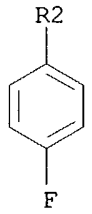
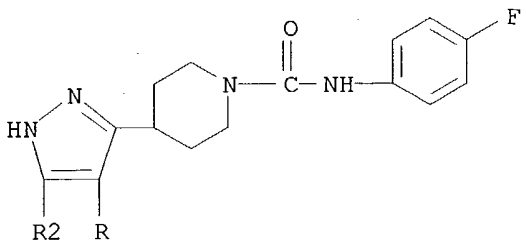
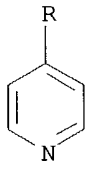


RN 216525-02-9 CAPLUS
CN 1-Piperidinecarboxamide, N-(4-fluorophenyl)-4-[5-(4-fluorophenyl)-4-(4-pyridinyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

PAGE 1-A





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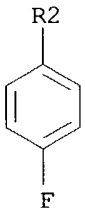

RN 216525-57-4 CAPLUS
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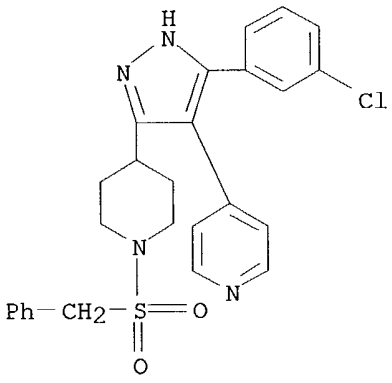
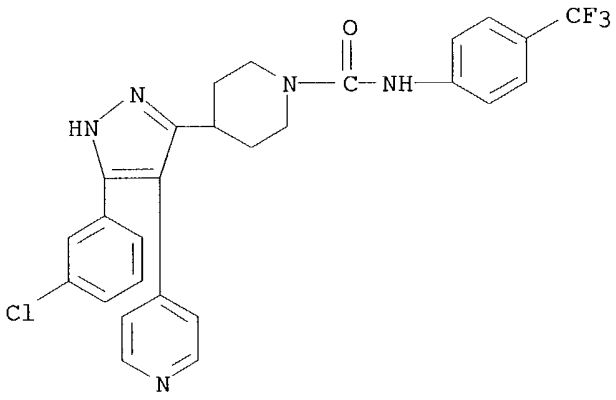
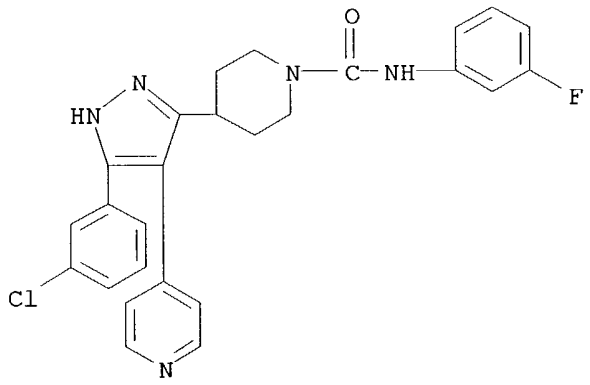


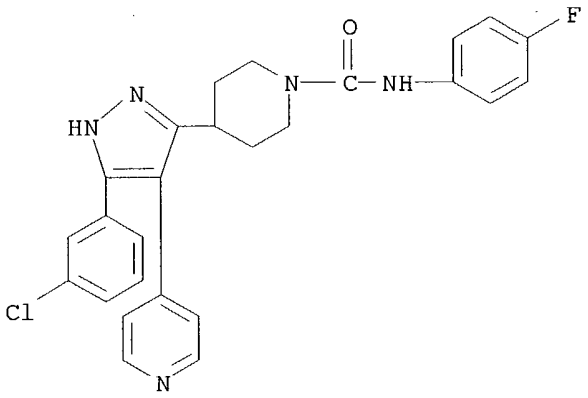
RN 216525-69-8 CAPLUS
CN 1-Piperidinecarboxamide, 4-[5-(3-chlorophenyl)-4-(4-pyridinyl)-1H-pyrazol-3-yl]-N-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



RN 216525-71-2 CAPLUS
CN 1-Piperidinecarboxamide, 4-[5-(3-chlorophenyl)-4-(4-pyridinyl)-1H-pyrazol-3-yl]-N-(3-fluorophenyl)- (9CI) (CA INDEX NAME)

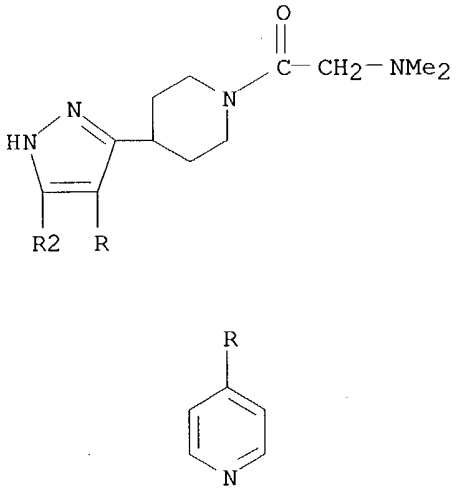


RN 216525-72-3 CAPLUS
CN 1-Piperidinecarboxamide, 4-[5-(3-chlorophenyl)-4-(4-pyridinyl)-1H-pyrazol-3-yl]-N-(4-fluorophenyl)- (9CI) (CA INDEX NAME)



RN 271576-62-6 CAPLUS
CN Piperidine, 4-[5-(4-chlorophenyl)-4-(4-pyridinyl)-1H-pyrazol-3-yl]-1-[(dimethylamino)acetyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



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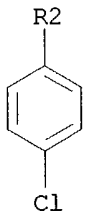

RE.CNT 76 THERE ARE 76 CITED REFERENCES AVAILABLE FOR THIS RECORD

L4 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:832793 CAPLUS
DN 137:337886
TI Preparation of pyrazolyl- and isoxazolylpyridinium halides for treatment of aging-related and diabetic vascular complications
IN Sankaranarayanan, Alangudi
PA India
SO PCT Int. Appl., 180 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002085897	A1	20021031	WO 2002-IB1137	20020402
	WO 2002085897	C1	20021128		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
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	EP 1373263	A1	20040102	EP 2002-722547	20020402
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	US 2003045554	A1	20030306	US 2002-116135	20020405
PRAI	US 2001-281380P	P	20010405		
	WO 2002-IB1137	W	20020402		

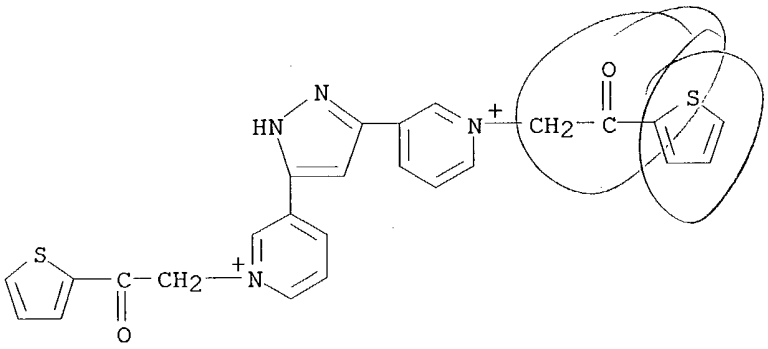
OS MARPAT 137:337886
AB Title compds. I.bul.X- [wherein R1 = H or (un)substituted (heterocyclo)alkyl, alkenyl, (bi)cycloalkyl, (bi)cycloalkenyl, (hetero)aryl, or (hetero)aralkyl; Y = alkyl-Z or alkyl; Z = S, O, or N; A and B = independently NH, NR6, S, O, or C; R2, R3, and R4 = independently H, halo, NO2, N:CR8R9, NR8R9, OR8, perhaloalkyl, CONR7R9, COR8, CO2R8, OCOR8, NHCOR8, or (un)substituted (heterocyclo)alkyl, alkenyl, (bi)cycloalkyl, (bi)cycloalkenyl, (hetero)aryl, or (hetero)aralkyl; R5 = null or (un)substituted (cyclo)alkyl, (cyclo)alkenyl, bicycloalkyl, CH2COR7, CH2CONHR8, CH2CONR8R9, or CH2CO2R7; R6 and R7 = independently (un)substituted alkyl, perhalo(cyclo)alkyl, (alkyl)cycloalkyl, (hetero)aryl, (hetero)aralkyl, alkyl(hetero)aryl, aralkoxyalkyl, acyl, benzoyl, alkoxyalkyl, thioalkyl, thioaryl, etc.; R8 and R9 = independently (un)substituted (perhalo)alkyl, (perhalo)cycloalkyl, alkoxy(cyclo)alkyl, alkoxyaryl, heterocycloalkyl, etc.; and pharmaceutically or cosmetically acceptable salts thereof] were prepd. I.bul.X- act by triple action of an AGE (advanced glycation endproducts) breaker, AGE inhibitor, and free radical scavenger. For example, 3-acetylpyridine was added to Et 3,5-dimethylpyrazolylacetate to give the butane-1,3-dione, which was then cyclized with hydrazine in MeOH to afford 3-[3-(3,5-dimethylpyrazol-1-ylmethyl)pyrazol-5-yl]pyridine. Quaternization with .alpha.-bromo-2-acetylthiophene in IPA produced the pyridinium bromide (II.bul.Br-). Representative compds. of the invention exhibited AGE breaking activity between 42.37% and 100% at concns. of 10 mM, inhibited AGE activity between 55.22% and 82.5% at concns. of 5 mM, and displayed free radical scavenging activity on ABTS between 29.40% and 99.71% at concns. of 100

.mu.M. Thus, I.bul.X- are useful for therapeutic and cosmetic applications, particularly in the management of aging-related and diabetic vascular complications (no data). Pharmaceuticals and cosmetic compns. comprising I are also disclosed.

IT **473881-95-7P**, 3,5-Bis[1-[2-(thien-2-yl)-2-oxoethyl]pyridinium-3-yl]pyrazole dibromide
RL: COS (Cosmetic use); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(AGE inhibitor; prepn. of pyrazolyl- and isoxazolylpyridinium halide AGE inhibitors by formation of diketo compds., cyclization, and quaternization)

RN 473881-95-7 CAPLUS

CN Pyridinium, 3,3'-(1H-pyrazole-3,5-diyl)bis[1-[2-oxo-2-(2-thienyl)ethyl]-, dibromide (9CI) (CA INDEX NAME)



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RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2000:368337 CAPLUS
DN 133:4656
TI Preparation of heteroarylpyrazoles as p38 kinase inhibitors
IN Anantanarayan, Ashok; Clare, Michael; Collins, Paul W.; Crich, Joyce Z.; Devraj, Rajesh; Flynn, Daniel L.; Geng, Lifeng; Graneto, Matthew J.; Hanau, Cathleen E.; Hanson, Gunnar J.; Hartmann, Susan J.; Hepperle, Michael; Huang, He; Khanna, Ish K.; Koszyk, Francis J.; Liao, Shuyuan; Metz, Suzanne; Partis, Richard A.; Perry, Thao D.; Rao, Shashidhar N.; Selness, Shaun Raj; South, Michael S.; Stealey, Michael A.; Talley, John Jeffrey; Vazquez, Michael L.; Weier, Richard M.; Xu, Xiangdong; Yu, Yi
PA G.D. Searle and Co., USA
SO PCT Int. Appl., 1210 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 4

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000031063	A1	20000602	WO 1999-US26007	19991117
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	RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	US 6514977	B1	20030204	US 1998-196623	19981120
	EP 1144403	A1	20011017	EP 1999-965756	19991117
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	BR 9915420	A	20020122	BR 1999-15420	19991117
	EE 200100268	A	20021216	EE 2001-268	19991117
	NZ 512344	A	20031128	NZ 1999-512344	19991117
	US 6525059	B1	20030225	US 2000-513351	20000224
	NO 2001002456	A	20010719	NO 2001-2456	20010518
	BG 105620	A	20020131	BG 2001-105620	20010619
PRAI	US 1998-196623	A	19981120		
	US 1997-47570P	P	19970522		
	US 1998-83670	A2	19980522		
	WO 1999-US26007	W	19991117		

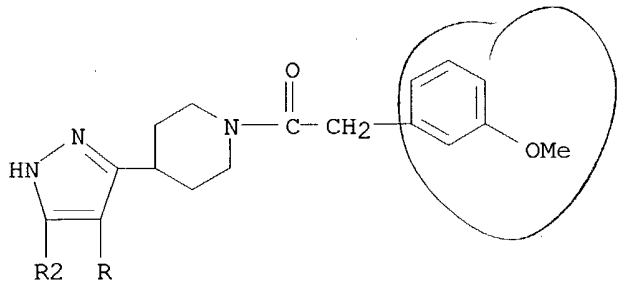
OS MARPAT 133:4656
AB Title compds. [I; R1 = H, OH, NH2, (cyclo)alk(en)yl, acyl, aryl, etc.; R2 = H, halo, alkyl, alkoxy, (un)substituted piperidinyl, etc.; R3 = pyridyl, pyrimidinyl, quinolyl, etc.; R4 = H, alkyl, heterocyclyl, aryl, etc.] were prepd. by reaction of ketones with hydrazines. Thus, R3CH2COMe (R3 = 4-pyridinyl) was condensed with 3,4-F(MeO)C6H3CHO and the product cyclocondensed with TsNHNH2 to give title compd. II. Data for biol. activity of I were given.
IT **216523-75-0P 216523-79-4P 216523-84-1P**
216523-85-2P 216523-87-4P 216524-32-2P
216524-96-8P 216525-00-7P 216525-02-9P
216525-57-4P 216525-69-8P 216525-71-2P
216525-72-3P 271576-62-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);

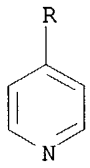
BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of heteroarylpyrazole p38 kinase inhibitors by cyclocondensation of hydrazines with ketones)

RN 216523-75-0 CAPLUS

CN Piperidine, 4-[5-(4-fluorophenyl)-4-(4-pyridinyl)-1H-pyrazol-3-yl]-1-[(3-methoxyphenyl)acetyl]- (9CI) (CA INDEX NAME)

PAGE 1-A





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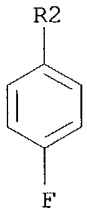
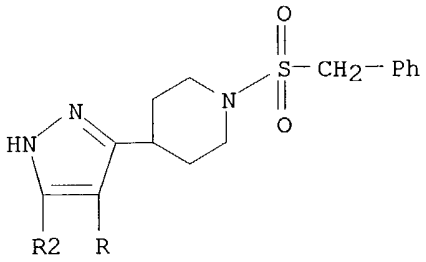
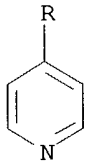


RN 216523-79-4 CAPLUS

CN Piperidine, 4-[5-(4-fluorophenyl)-4-(4-pyridinyl)-1H-pyrazol-3-yl]-1-[(phenylmethyl)sulfonyl]- (9CI) (CA INDEX NAME)

PAGE 1-A





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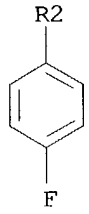
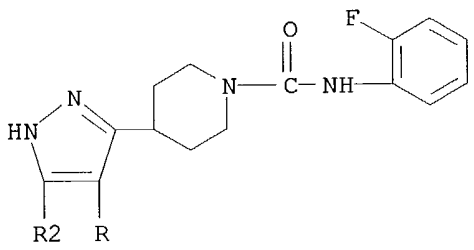
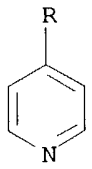


RN 216523-84-1 CAPLUS
CN 1-Piperidinecarboxamide, N-(2-fluorophenyl)-4-[5-(4-fluorophenyl)-4-(4-pyridinyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

PAGE 1-A





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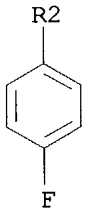
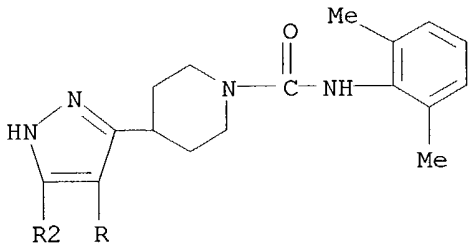
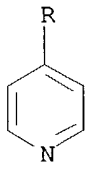


RN 216523-85-2 CAPLUS
CN 1-Piperidinecarboxamide, N-(2,6-dimethylphenyl)-4-[5-(4-fluorophenyl)-4-(4-pyridinyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

PAGE 1-A





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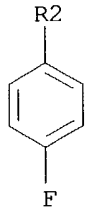
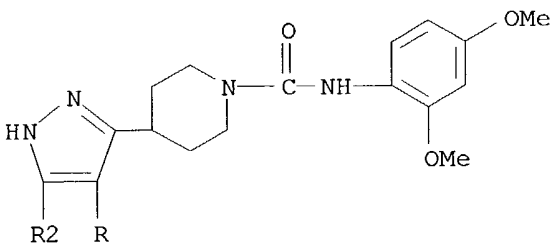
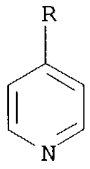


RN 216523-87-4 CAPLUS
CN 1-Piperidinecarboxamide, N-(2,4-dimethoxyphenyl)-4-[5-(4-fluorophenyl)-4-(4-pyridinyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

PAGE 1-A

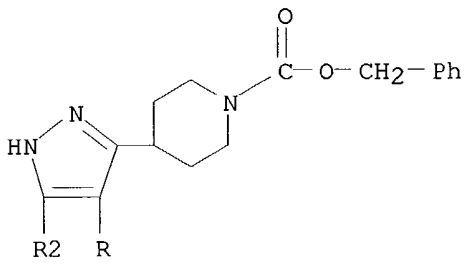


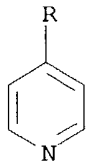


PAGE 2-A

RN 216524-32-2 CAPLUS
CN 1-Piperidinecarboxylic acid, 4-[5-(4-fluorophenyl)-4-(4-pyridinyl)-1H-pyrazol-3-yl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A





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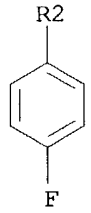
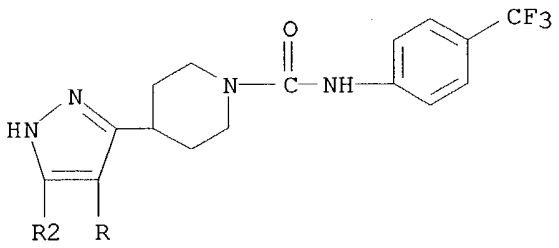
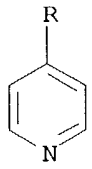


RN 216524-96-8 CAPLUS
CN 1-Piperidinecarboxamide, 4-[5-(4-fluorophenyl)-4-(4-pyridinyl)-1H-pyrazol-3-yl]-N-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

PAGE 1-A





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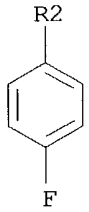

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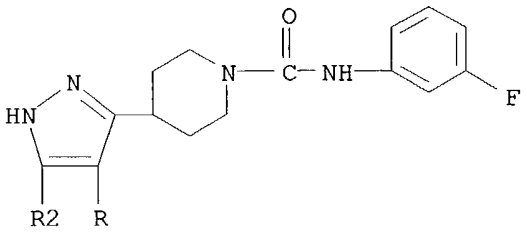
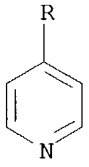
CN 1-Piperidinecarboxamide, N-(3-fluorophenyl)-4-[5-(4-fluorophenyl)-4-(4-pyridinyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

PAGE 1-A





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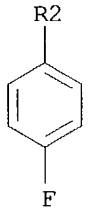

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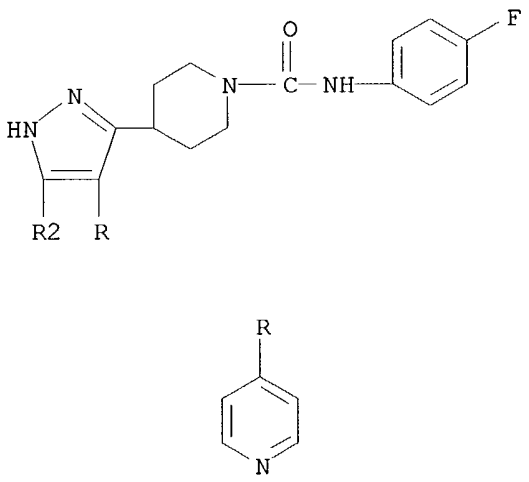
CN 1-Piperidinecarboxamide, N-(4-fluorophenyl)-4-[5-(4-fluorophenyl)-4-(4-pyridinyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

PAGE 1-A



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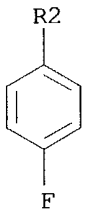

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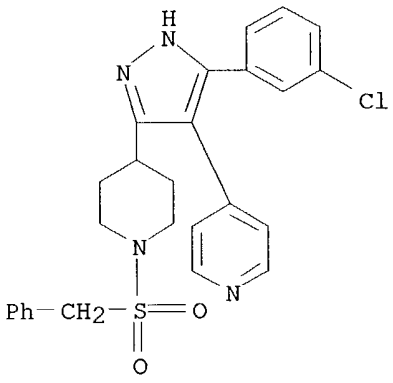
CN Piperidine, 4-[5-(3-chlorophenyl)-4-(4-pyridinyl)-1H-pyrazol-3-yl]-1-[(phenylmethyl)sulfonyl]- (9CI) (CA INDEX NAME)



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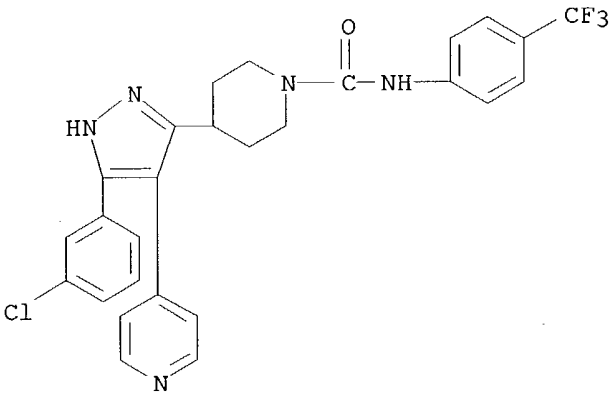

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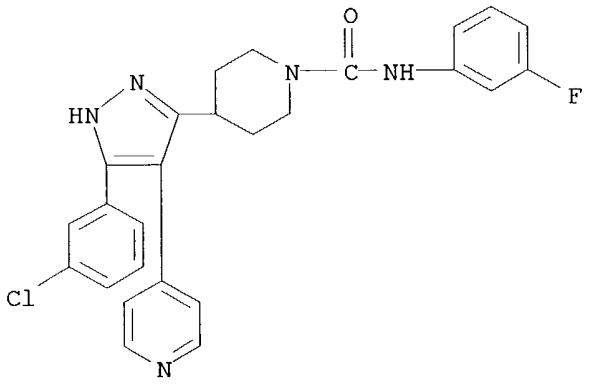

RN 216525-72-3 CAPLUS
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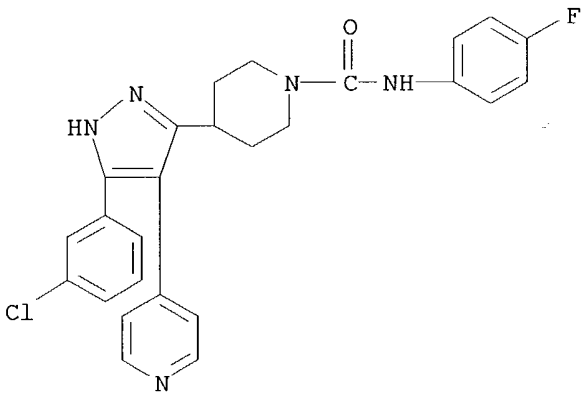

RN 271576-62-6 CAPLUS
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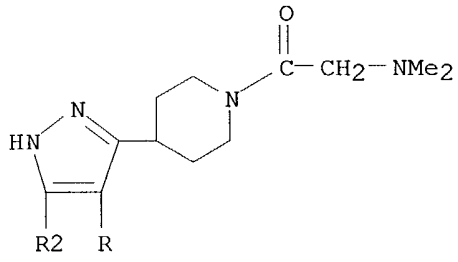
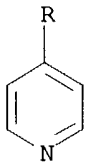
PAGE 1-A





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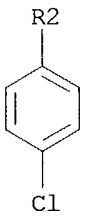

RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD

L4 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1998:789144 CAPLUS
DN 130:38377
TI Preparation of heteroarylpyrazoles as p38 kinase inhibitors
IN Anantanarayan, Ashok; Clare, Michael; Collins, Paul W.; Crich, Joyce Zuowu; Devraj, Rajesh; Flynn, Daniel L.; Geng, Lifeng; Hanson, Gunnar J.; Koszyk, Francis J.; Liao, Shuyuan; Partis, Richard A.; Rao, Shashidhar N.; Selness, Shaun Raj; South, Michael S.; Stealey, Michael A.; Weier, Richard M.; Xu, Xiangdong
PA G.D. Searle and Co., USA; et al.
SO PCT Int. Appl., 828 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 4

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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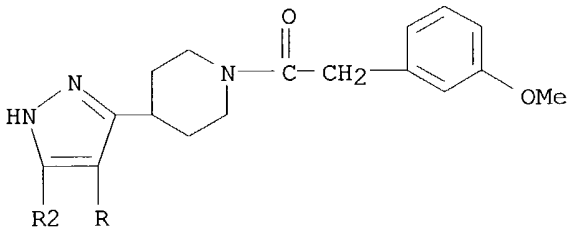
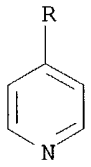
PRAI	US 1997-47570P	P	19970522		
	WO 1998-US10436	W	19980522		

OS MARPAT 130:38377
AB Title compds. [I; R1 = H, NH2, (cyclo)alk(en)yl, acyl, aryl, etc.; R2 = H, halo, alkyl, alkoxy, etc.; R3 = pyridyl, pyrimidinyl, quinolyl, etc.; R4 = H, alkyl, heterocyclyl, aryl, etc.] were prepd. Thus, R3CH2COMe (R3 = 4-pyridinyl) was condensed with 3,4-F(MeO)C6H3CHO and the product cyclocondensed with TsNHNH2 to give title compd. II. Data for biol. activity of I were given.
IT **216523-75-0P 216523-79-4P 216523-84-1P**
216523-85-2P 216523-87-4P 216524-32-2P
216524-96-8P 216525-00-7P 216525-02-9P
216525-57-4P 216525-69-8P 216525-71-2P
216525-72-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of heteroarylpyrazoles as p38 kinase inhibitors)
RN 216523-75-0 CAPLUS
CN Piperidine, 4-[5-(4-fluorophenyl)-4-(4-pyridinyl)-1H-pyrazol-3-yl]-1-[(3-

methoxyphenyl)acetyl]- (9CI) (CA INDEX NAME)

PAGE 1-A





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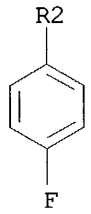

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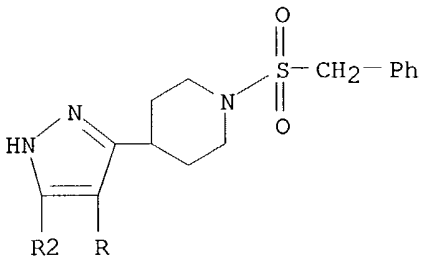
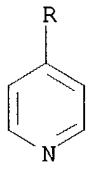
PAGE 1-A





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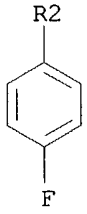

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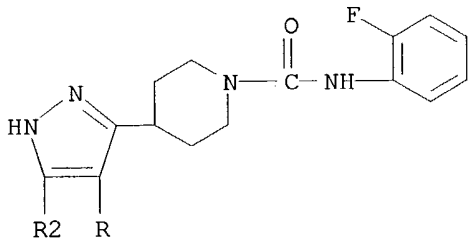
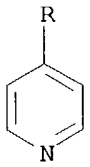
CN 1-Piperidinecarboxamide, N-(2-fluorophenyl)-4-[5-(4-fluorophenyl)-4-(4-pyridinyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

PAGE 1-A





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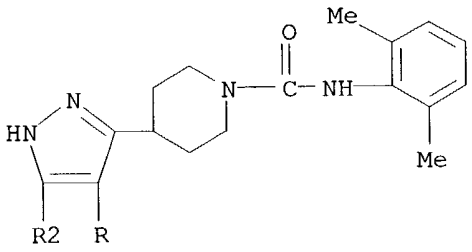
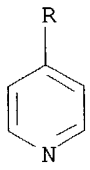
RN 216523-85-2 CAPLUS
CN 1-Piperidinecarboxamide, N-(2,6-dimethylphenyl)-4-[5-(4-fluorophenyl)-4-(4-pyridinyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

PAGE 1-A





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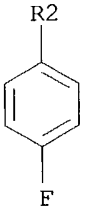

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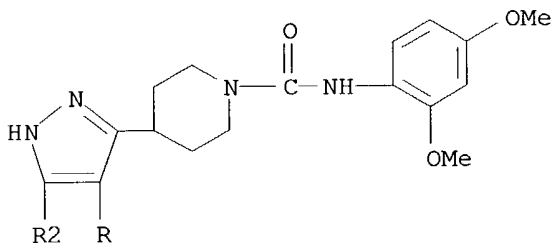
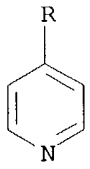
CN 1-Piperidinecarboxamide, N-(2,4-dimethoxyphenyl)-4-[5-(4-fluorophenyl)-4-(4-pyridinyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

PAGE 1-A





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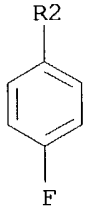
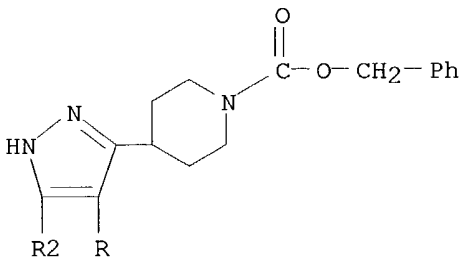
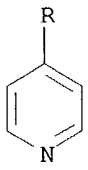


RN 216524-32-2 CAPLUS
CN 1-Piperidinecarboxylic acid, 4-[5-(4-fluorophenyl)-4-(4-pyridinyl)-1H-pyrazol-3-yl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A





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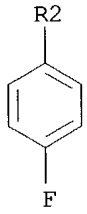

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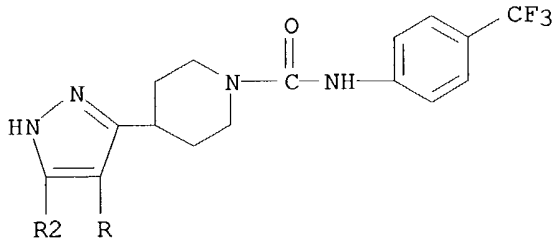
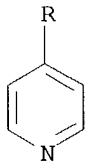
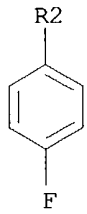
CN 1-Piperidinecarboxamide, 4-[5-(4-fluorophenyl)-4-(4-pyridinyl)-1H-pyrazol-3-yl]-N-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



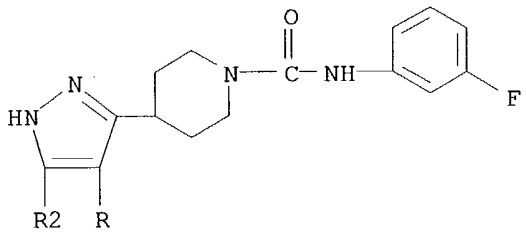


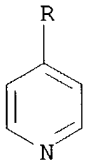
PAGE 2-A



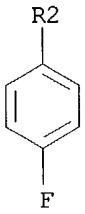
RN 216525-00-7 CAPLUS
CN 1-Piperidinecarboxamide, N-(3-fluorophenyl)-4-[5-(4-fluorophenyl)-4-(4-pyridinyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

PAGE 1-A



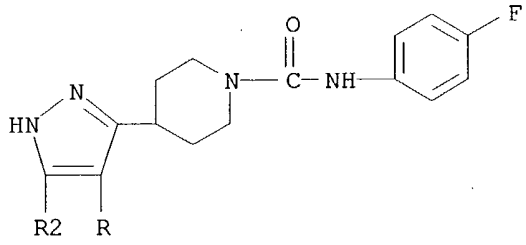


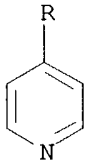
PAGE 2-A



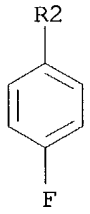
RN 216525-02-9 CAPLUS
CN 1-Piperidinecarboxamide, N-(4-fluorophenyl)-4-[5-(4-fluorophenyl)-4-(4-pyridinyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

PAGE 1-A

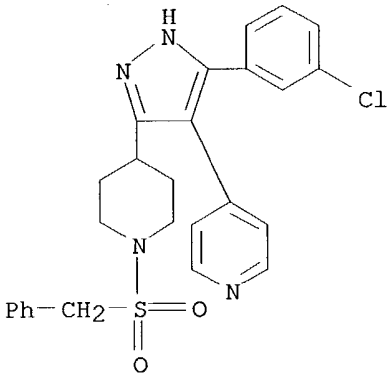




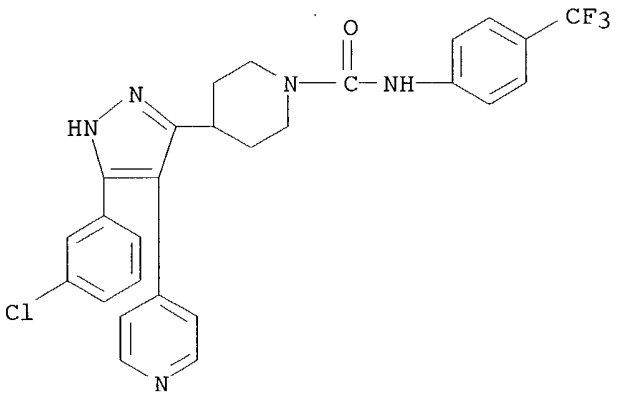
PAGE 2-A



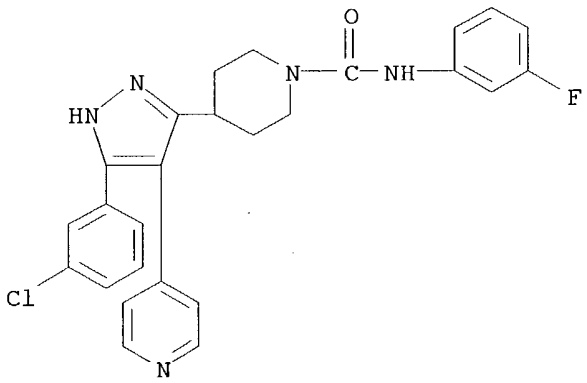
RN 216525-57-4 CAPLUS
CN Piperidine, 4-[5-(3-chlorophenyl)-4-(4-pyridinyl)-1H-pyrazol-3-yl]-1-[(phenylmethyl)sulfonyl]- (9CI) (CA INDEX NAME)



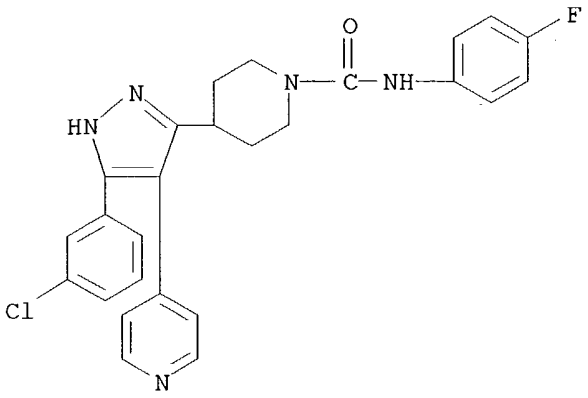
RN 216525-69-8 CAPLUS
CN 1-Piperidinecarboxamide, 4-[5-(3-chlorophenyl)-4-(4-pyridinyl)-1H-pyrazol-3-yl]-N-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



RN 216525-71-2 CAPLUS
CN 1-Piperidinecarboxamide, 4-[5-(3-chlorophenyl)-4-(4-pyridinyl)-1H-pyrazol-3-yl]-N-(3-fluorophenyl)- (9CI) (CA INDEX NAME)

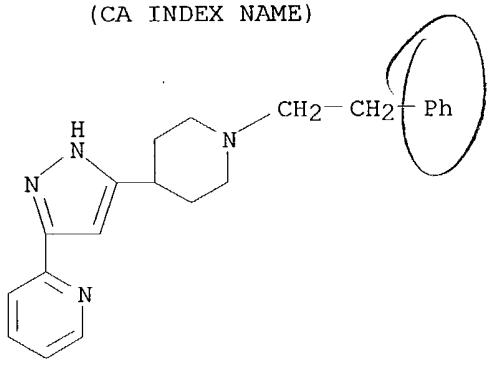


RN 216525-72-3 CAPLUS
CN 1-Piperidinecarboxamide, 4-[5-(3-chlorophenyl)-4-(4-pyridinyl)-1H-pyrazol-3-yl]-N-(4-fluorophenyl)- (9CI) (CA INDEX NAME)

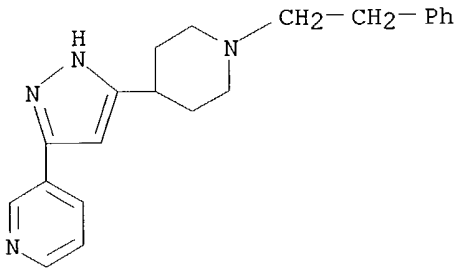


RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

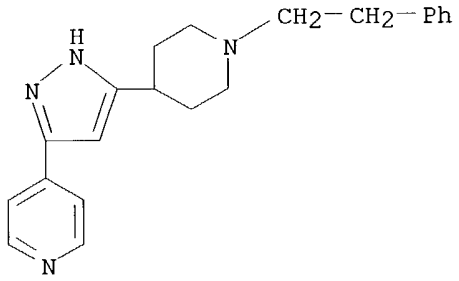
L4 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1997:436020 CAPLUS
DN 127:81332
TI 4-Heterocyclylpiperidines as Selective High-Affinity Ligands at the Human Dopamine D4 Receptor
AU Rowley, Michael; Collins, Ian; Broughton, Howard B.; Davey, William B.; Baker, Raymond; Emms, Frances; Marwood, Rosemarie; Patel, Shil; Patel, Smita; Ragan, C. Ian; Freedman, Stephen B.; Ball, Richard; Leeson, Paul D.
CS Neuroscience Research Centre, Merck Sharp and Dohme, Harlow/Essex, CM20 2QR, UK
SO Journal of Medicinal Chemistry (1997), 40(15), 2374-2385
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
AB 5-(4-Chlorophenyl)-3-(1-(4-chlorobenzyl)piperidin-4-yl)pyrazole was identified from screening of the Merck sample collection as a human dopamine D4 (hD4) receptor ligand with moderate affinity (61 nM) and 4-fold selectivity over human D2 (hD2) receptors. Four sep. parts of the mol. have been examd. systematically to explore structure-activity relationships with respect to hD4 affinity and selectivity over other dopamine receptors. It was found that the 4-chlorophenyl group attached to the pyrazole is optimal, as is the 4-substituted piperidine. The lipophilic group on the basic nitrogen is more amenable to change, with the optimal group found to be a phenethyl. The arom. heterocycle can be altered to a no. of different groups, with isoxazoles and pyrimidines showing improved affinities. This heterocycle can also be advantageously alkylated, improving the selectivity of the compds. over D2 receptors. It is hypothesized that the conformation around the bond joining the arom. heterocycle to the piperidine is important for D4 affinity. Putting all the favorable changes together led to the discovery that 5-(4-chlorophenyl)-4-methyl-3-(1-(2-phenylethyl)piperidin-4-yl)isoxazole (I) is a nanomolar antagonist at human dopamine D4 receptors with >500-fold selectivity over hD2 and >200-fold selectivity over hD3. I is an antagonist of hD4 receptors with good oral bioavailability of 38%, a half life of 2 h, and brain levels 10-fold higher than plasma levels.
IT **156337-22-3P 184374-56-9P 184374-60-5P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. of heterocyclylpiperidines as selective high-affinity ligands at the human dopamine D4 receptor)
RN 156337-22-3 CAPLUS
CN Pyridine, 2-[5-[1-(2-phenylethyl)-4-piperidinyl]-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



RN 184374-56-9 CAPLUS
CN Pyridine, 3-[5-[1-(2-phenylethyl)-4-piperidinyl]-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



RN 184374-60-5 CAPLUS
CN Pyridine, 4-[5-[1-(2-phenylethyl)-4-piperidinyl]-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

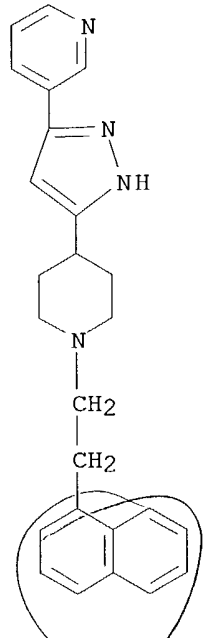


L4 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1996:751643 CAPLUS
DN 126:31349
TI Use of pyrazolylpiperidine derivatives as alpha 1a adrenergic receptor antagonists, for treatment of benign prostatic hypertrophy.
IN Payne, Linda S.; Young, Steven D.; Zaborowski, Mary Jo L.
PA Merck and Co., Inc., USA; Payne, Linda S.; Young, Steven D.; Zaborowski, Mary Jo L.
SO PCT Int. Appl., 94 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

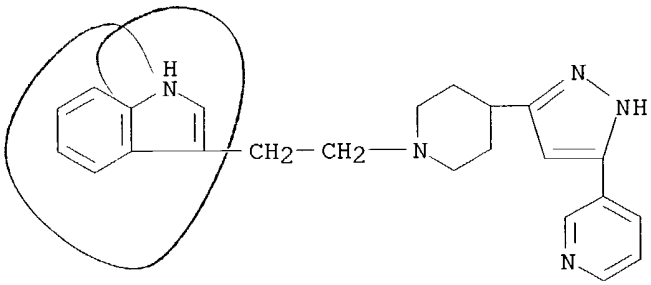
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9632938	A1	19961024	WO 1996-US5251	19960416
	W: AL, AM, AU, AZ, BB, BG, BR, BY, CA, CN, CZ, EE, GE, HU, IS, JP, KG, KR, KZ, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, TT, UA, US, UZ, VN, AM, AZ, BY, KG, KZ, MD				
	RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	US 5668148	A	19970916	US 1995-425969	19950420
	CA 2218391	AA	19961024	CA 1996-2218391	19960416
	AU 9655495	A1	19961107	AU 1996-55495	19960416
	AU 706092	B2	19990610		
	EP 822814	A1	19980211	EP 1996-912805	19960416
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
	JP 11504010	T2	19990406	JP 1996-531850	19960416
PRAI	US 1995-425969		19950420		
	WO 1996-US5251		19960416		

OS MARPAT 126:31349
AB Compds. that specifically bind to the human .alpha.1a adrenergic receptor (no data), including compds. which are effective for reducing symptoms of benign prostatic hypertrophy, include compds. I [Ar1, Ar2 = arom., heteroarom., or condensed heteroarom. rings, (un)substituted with amino, alkoxy, sulfonamido, alkyl, heteroalkyl, halo; m = 0 or 1; n = 0, 1, or 2; het = arom. or nonarom. heterocyclic ring, substituted with alkyl, halo, or alkoxy substituents; and X = branched or straight chain aliph. or halo]. Over 30 target compds. were prepd., and the use of these and approx. 70 addnl. compds. is claimed. For example, 3-acetylpyridine was lithiated with LDA, and the product enolate reacted with the imidazolide of Boc-isonipecotic acid (prepd. using 1,1'-carbonyldiimidazole) to give intermediate II. This underwent deprotection with dry HCl in EtOAc, N-alkylation with 1-(2-bromoethyl)naphthalene, and cyclocondensation with hydrazine, to give title compd. III.
IT **184373-98-6P 184373-99-7P 184374-11-6P**
184374-19-4P 184374-20-7P 184374-21-8P
184374-22-9P 184374-23-0P 184374-24-1P
184374-25-2P 184374-26-3P 184374-32-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. and use of pyrazolylpiperidine derivs. as .alpha.1a-adrenergic receptor antagonists)
RN 184373-98-6 CAPLUS
CN Pyridine, 3-[5-[1-[2-(1-naphthalenyl)ethyl]-4-piperidinyl]-1H-pyrazol-3-

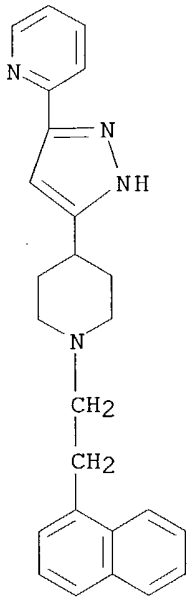
yl]- (9CI) (CA INDEX NAME)



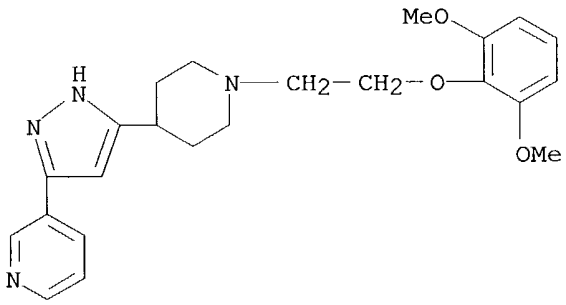
RN 184373-99-7 CAPLUS
CN 1H-Indole, 3-[2-[4-[5-(3-pyridinyl)-1H-pyrazol-3-yl]-1-piperidinyl]ethyl]- (9CI) (CA INDEX NAME)



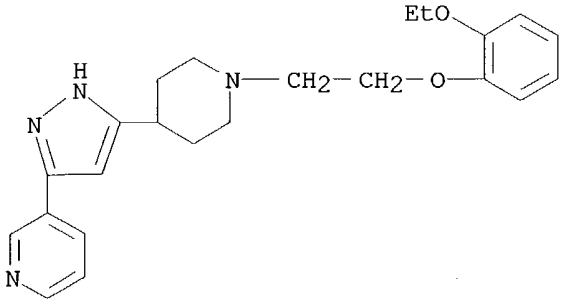
RN 184374-11-6 CAPLUS
CN Pyridine, 2-[5-[1-[2-(1-naphthalenyl)ethyl]-4-piperidinyl]-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



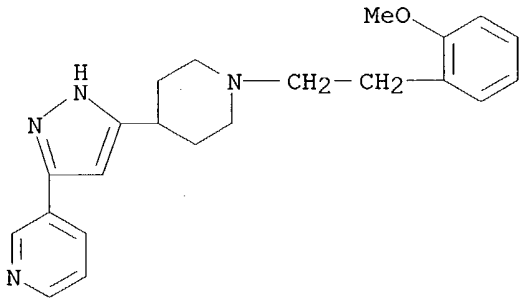
RN 184374-19-4 CAPLUS
CN Pyridine, 3-[5-[1-[2-(2,6-dimethoxyphenoxy)ethyl]-4-piperidinyl]-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



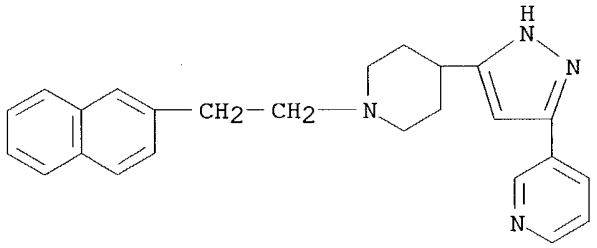
RN 184374-20-7 CAPLUS
CN Pyridine, 3-[5-[1-[2-(2-ethoxyphenoxy)ethyl]-4-piperidinyl]-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



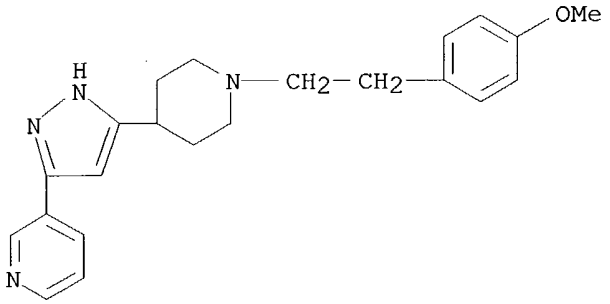
RN 184374-21-8 CAPLUS
CN Pyridine, 3-[5-[1-[2-(2-methoxyphenyl)ethyl]-4-piperidinyl]-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



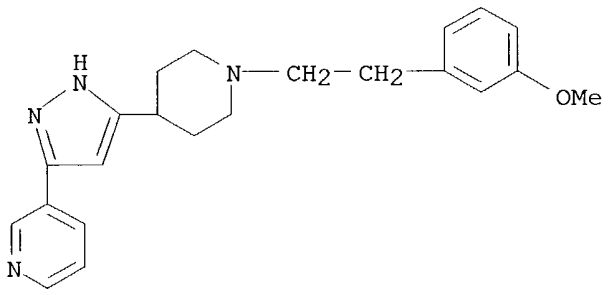
RN 184374-22-9 CAPLUS
CN Pyridine, 3-[5-[1-[2-(2-naphthalenyl)ethyl]-4-piperidinyl]-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



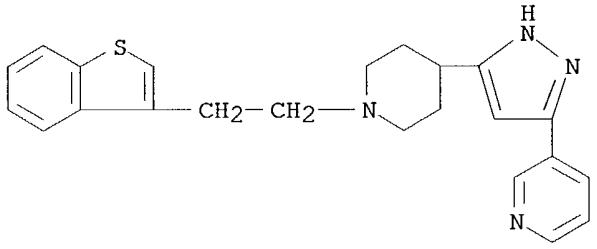
RN 184374-23-0 CAPLUS
CN Pyridine, 3-[5-[1-[2-(4-methoxyphenyl)ethyl]-4-piperidinyl]-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



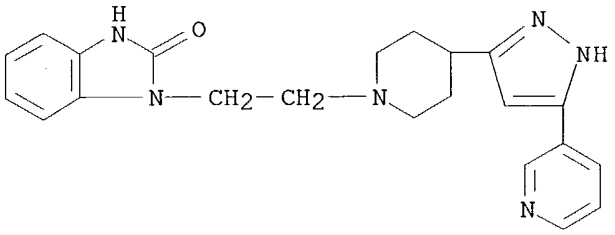
RN 184374-24-1 CAPLUS
CN Pyridine, 3-[5-[1-[2-(3-methoxyphenyl)ethyl]-4-piperidinyl]-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



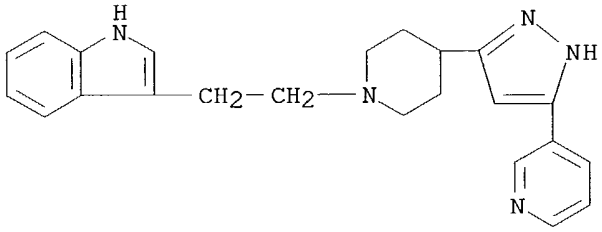
RN 184374-25-2 CAPLUS
CN Pyridine, 3-[5-[1-(2-benzo[b]thien-3-ylethyl)-4-piperidinyl]-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



RN 184374-26-3 CAPLUS
CN 2H-Benzimidazol-2-one, 1,3-dihydro-1-[2-[4-[5-(3-pyridinyl)-1H-pyrazol-3-yl]-1-piperidinyl]ethyl]- (9CI) (CA INDEX NAME)

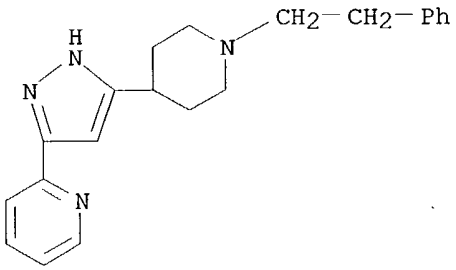


RN 184374-32-1 CAPLUS
CN 1H-Indole, 3-[2-[4-[5-(3-pyridinyl)-1H-pyrazol-3-yl]-1-piperidinyl]ethyl]-, dihydrochloride (9CI) (CA INDEX NAME)

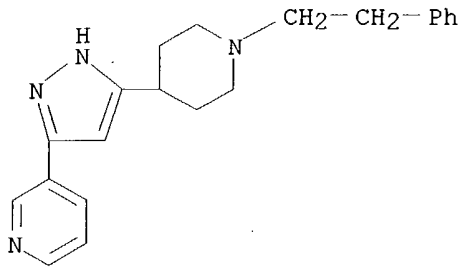


●2 HCl

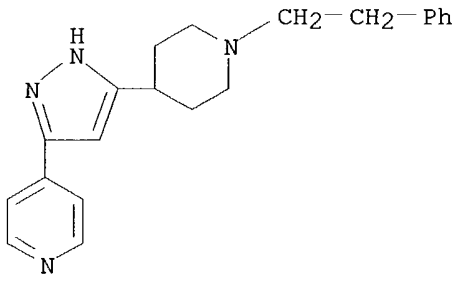
IT **156337-22-3 184374-56-9 184374-60-5**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(prepn. and use of pyrazolylpiperidine derivs. as .alpha.1a-adrenergic receptor antagonists)
RN 156337-22-3 CAPLUS
CN Pyridine, 2-[5-[1-(2-phenylethyl)-4-piperidinyl]-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



RN 184374-56-9 CAPLUS
CN Pyridine, 3-[5-[1-(2-phenylethyl)-4-piperidinyl]-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



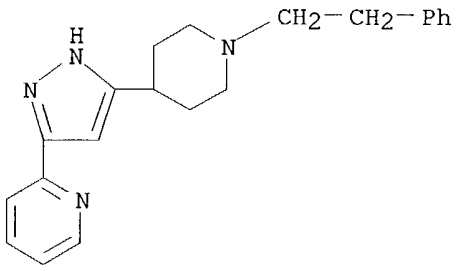
RN 184374-60-5 CAPLUS
CN Pyridine, 4-[5-[1-(2-phenylethyl)-4-piperidinyl]-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



L4 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1994:483041 CAPLUS
DN 121:83041
TI (Piperidinyl)pyrazoles and Analogs as Dopamine Receptor Subtype Ligands
IN Broughton, Howard Barff; Collins, Ian James; Baker, Raymond; Leeson, Paul David; Rowley, Michael
PA Merck Sharp and Dohme Ltd., UK
SO PCT Int. Appl., 76 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9410145	A1	19940511	WO 1993-GB2190	19931022
	W: AU, CA, JP, US				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	CA 2146019	AA	19940511	CA 1992-2146019	19931022
	AU 9453414	A1	19940524	AU 1994-53414	19931022
	AU 678186	B2	19970522		
	EP 665833	A1	19950809	EP 1993-923608	19931022
	EP 665833	B1	19990714		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
	JP 08502508	T2	19960319	JP 1993-510809	19931022
	AT 182139	E	19990715	AT 1993-923608	19931022
	ES 2133416	T3	19990916	ES 1993-923608	19931022
	US 5631269	A	19970520	US 1995-424364	19950420
PRAI	GB 1992-22263		19921023		
	GB 1992-22265		19921023		
	WO 1993-GB2190		19931022		

OS MARPAT 121:83041
AB Pyrazoles and oxazoles and thiazoles I (X, Y = N, the other of X, Y = O, S, N; Q = heterocyclic ring; A = substituted Ph, pyridinyl, thioenyl, etc.; R1 = H, halo, alkyl, etc.) were disclosed. I are ligands for dopamine receptor subtypes within the body and are therefore useful in the treatment of disorders of the dopamine system, in particular schizophrenia. An example compd., 1-(4-chlorophenyl)-[5-(4-chlorophenyl)-1H-pyrazol-3-yl]piperidine (II) was prepd. Pharmacol. test data for I were not presented.
IT **156337-22-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as antischizophrenic)
RN 156337-22-3 CAPLUS
CN Pyridine, 2-[5-[1-(2-phenylethyl)-4-piperidinyl]-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



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L3           31 S L1 SSS FUL

     FILE 'CAPLUS' ENTERED AT 18:01:13 ON 03 FEB 2004
L4           10 S L3

     FILE 'CAOLD' ENTERED AT 18:01:52 ON 03 FEB 2004

=> s l3
L5            0 L3

=> log y
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